OTAVA chemicals

Compounds for HTS
Chemical building blocks
Fragment libraries
Targeted libraries
Drug discovery services

FUNGICIDES-LIKE LIBRARY

OTAVA chemicals

OTAVA offers Fungicides-Like Library - special screening library containing predicted fungicides. This library provides an excellent basis for fungicide discovery projects.

The library consists of **1,865 compounds***.

All compounds are:

- **in stock**; available amounts: 1 – 50 mg

QA/QC passed:

- minimal purity of compounds is **90%**;
- by **NMR** and/or **GC/LC/MS**
- **NMR spectra are available** upon request

Frendly packing services:

- **Cherry-picking is available**
- Supplied as dry powder or DMSO solution**
- Packaging in deep-well plates or barcoded vials***
- **Weighing out is free**

*Please note that the library does not contain known inhibitors. The compounds were selected with computational approach and are intended for screening projects

**there is additional fee for preparation of the solution

***4 ml amber glass vials or Deep-well plates: Matrix cat# 4247 (1.4 mL, Blank, Polypropylene, Round Bottom Tubes) w/CapMats. Or plates and vials provided by customer.

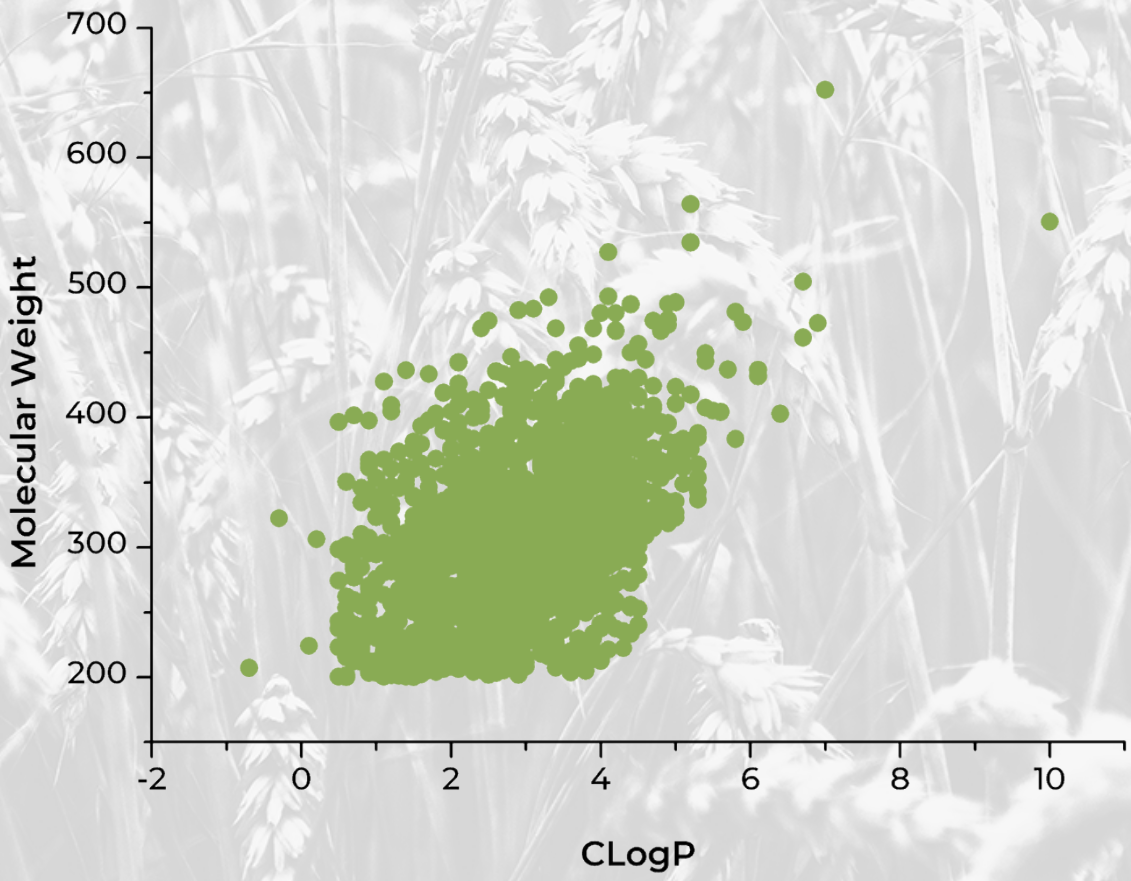
Target engagement:

Fungal pathogen comprises an important group of microorganisms that cause significant economic losses in agriculture around the world. Fungicides are chemical compounds used to kill fungi or fungal spores.

The summary of the library characteristics:

	Minimum	Maximum	Average value
Molecular Weight	200.2	652.2	311.7
Number of Hydrogen Bond Donors	0	4	0.9
Number of Hydrogen Bond Aceptors	1	10	4.3
Number of Rotatable Bonds	0	14	4
CLogP	-0.7	10	30
Number of Rings	0	7	2.5
Polar Surface Area	12	193.6	70.9

Distribution of physicochemical properties of compounds in the library:



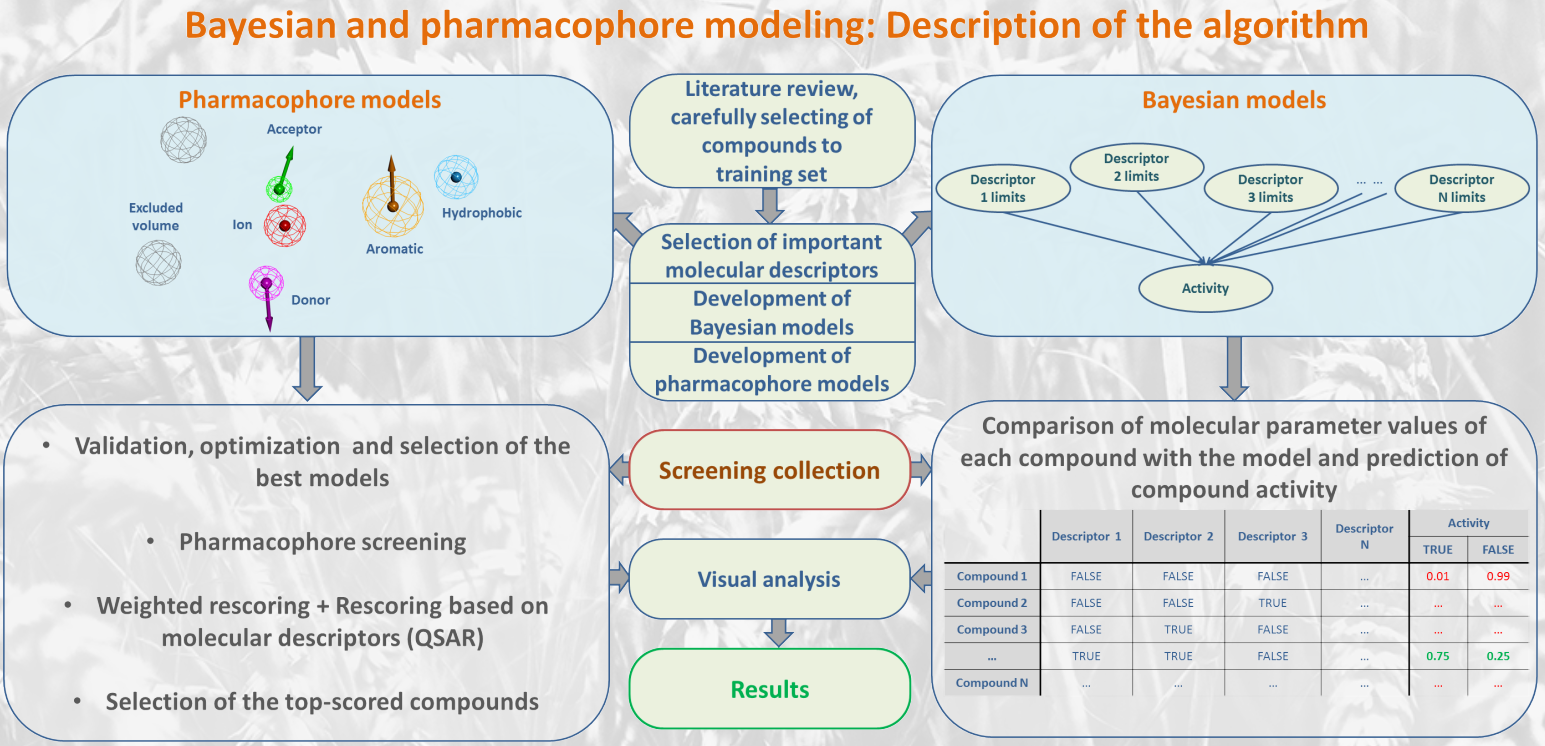
Design speciality:

Bayesian statistics and pharmacophore modeling combined with QSAR were used for development of it. The application of the combination of these methods and rescoring functions should allow increasing the number of active compounds identified during screening. (See Scheme 1)

Set of known fungicides was used for construction pharmacophore and Bayesian models. The four-poinf pharmacophore model with excluded volumes was developed, optimized, validated and OTAVA Screening Collection was screened against it. Obtained results were rescored using rescoring functions based on pharmacophore feature weightes and on molecular descriptors (QSAR) and visually analyzed.

Also Bayesian models were constructed for the same known fungicides based on FCFP4, FCFP6, ECFP4 and ECFP6 fingerprints and molecular descriptors such as LogP, molecular weight, number of rotatable bonds, number of hydrogen acceptors and donors, number of rings and molecular polar surface area. OTAVA Screening Collection was screened against them and top-scored compounds were selected.

Scheme 1. Bayesian and pharmacophore modeling: Description of the algorithm



OTAVA chemicals

Custom synthesis

Molecular modeling

Amyloids detection

Contract research

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